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Analysis of Different Approaches to Modeling of Nozzle Flows in the Near Continuum Regime (Preprint)

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Abstract. Conical nozzle flows are studied for Reynolds numbers of 1,230 and 12,300 using different numerical techniques: DSMC Method, Navier-Stokes/CFD accounting for velocity slip and temperature jump boundary conditions, and statistical and deterministic approaches to the solution of BGK equation. Detailed comparisons of the stability, accuracy, and convergence of the employed numerical techniques provides better understanding of their benefits and deficiencies, and assists in selecting the most appropriate technique for a particular nozzle and flow application. The deterministic and statistical solutions of the BGK equation were found to be in good agreement with the benchmark DSMC results. The Navier-Stokes solution differs from DSMC in the boundary layer.

Keywords: BGK Method, DSMC, low pressure case, high pressure case

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INTRODUCTION

Accurate and numerically efficient modeling of low and moderate Reynolds number nozzle flows is often problematic due to the existence of multiple flow length scales. Experimental studies of micro-nozzle based thrusters are rare, expensive, and may not provide the necessary precision in the measurement of principal nozzle characteristics such as thrust, flow rate, and specific impulse. The problem becomes even more severe when the influence of MEMS based thrusters on sensitive spacecraft surfaces needs to be analyzed. Back flow produced by such devices plays a major role in the contamination of sensitive electronic devices such as optical instruments, and solar panels etc., which in turn may adversely affect the life span of spacecraft. This back flow formation is sensitive to the flow conditions at the nozzle lip, and is also known to be difficult to study experimentally for such micro-nozzle flows [1].

The development of accurate numerical tools capable of handling micronozzle flows is therefore important, but challenging at the same time because the flow regime changes from continuum, near the nozzle throat, to transitional at the nozzle exit. Both kinetic methods, such as the Direct Simulation Monte Carlo (DSMC), and continuum, techniques based on Navier-Stokes (N-S) solutions, must meet computational and physical challenges when applied to these flows. The major problem with the DSMC method [2] is the associated computational cost when high density portions of the flow have to be accurately modeled. On the other hand, conventional continuum CFD techniques are inapplicable in the regions of high gradients and strong rarefaction even with the use

of velocity slip and temperature jump boundary conditions at the nozzle surface. It would therefore be highly desirable to have a single method that allows an accurate and efficient one-step modeling of high density nozzle and low density plume flows. To this end, the use of simplified forms of the Boltzmann equation, usually called model kinetic equations, such as Bhatnagar-Gross-Krook (BGK) may be useful [3]. A method based on BGK equation is expected to be more efficient than the DSMC method in the continuum and near-continuum regime, and more accurate than the solution of the N-S equations in the transition regime.

Recent years have witnessed a renewed interest and significant advances in the solution of model kinetic equations such as BGK, with deterministic, either finite difference or finite volume, approaches typically used in the solution procedure. A particle approach to obtain the solution to the BGK equation was first proposed in Ref. [4]. It was then extended to model the ES-BGK equation in Ref. [5], and further extended to include rotational degrees of freedom in Ref. [6]. The main goal of this paper is to apply statistical and deterministic approaches to obtain the solution of the BGK equation to simulate rarefied gas flow through a conical nozzle, and compare the results in terms of accuracy and efficiency to the solutions obtained with the traditional DSMC method and the Navier-Stokes equations. Four different numerical approaches - DSMC, finite volume and particle solutions of the BGK and ES-BGK model kinetic equations and an equilibrium DSMC (eDSMC) technique are used to study nozzle flows expanding into a vacuum.

GEOMETRY AND FLOW CONDITIONS

Gas flow of pure argon through a conical nozzle into vacuum is considered in this work. The diverging part of the nozzle is modeled, and its geometry is taken from Ref.[7]. The nozzle throat diameter is 2.5 mm, the length of the diverging part is 50.7 mm, and the half-angle is 20deg. The surface temperature of the nozzle is assumed to be 300 K. Numerical results are obtained for two throat-diameter based Reynolds numbers, 1,230 (Case I) and 12,300 (Case II), with the stagnation temperature of 333 K. In all numerical approaches, the computational domain starts at the nozzle throat and covers the entire diverging part of the nozzle, as well as a small part of the plume to avoid the influence of the downstream boundary conditions [8].

COMPUTATIONAL METHODS

DSMC method

The DSMC-based SMILE computational solver was used in this work. Details on the tool may be found in Ref. [9]. The SMILE features that were used in the present work include axisymmetric capability with radial weights, different grids for collisions and macroparameters, both of which are two-level adaptable Cartesian grids, and parallel implementation with efficient load balancing techniques. The majorant frequency scheme was employed for modeling molecular collisions in use of DSMC [10]. The VHS model was used for modeling molecular interactions. Diffuse reflection with full thermal accommodation was assumed on the nozzle wall. For both Reynolds numbers, solutions independent of grid, time step, and number of particles were obtained. For $Re=1,230$, there was virtually no difference observed between solutions obtained for 0.3 million cells with 1 million molecules, and 3 million cells with 10 million molecules. For $Re=12,300$, this was true for numerical parameters up to an order of magnitude larger. Tables 1 and 2 provide a summary of the numerical parameters for the two cases considered in this work.

Solution of NS equations

A commercial code, CFD++ [11] has been used in this work to solve the Navier-Stokes equations. CFD++ is a flexible CFD software suitable for the solution of steady/unsteady, compressible/incompressible N-S equations, including multi-species capability for perfect and reacting gases. In this work, a perfect-gas compressible N-S solver was used with second order spatial dis-

cretization and implicit time integration. Second order velocity slip and temperature jump conditions were imposed on the nozzle wall. A supersonic inflow with prescribed parameters was applied at the nozzle throat, and backpressure of 1 Pa was imposed at the outflow boundaries. The results presented in this paper were obtained for a multi-block rectangular grid with a total of 14,400 nodes. The computations were also conducted for four times smaller and four times larger numbers of nodes, and found to be fully grid-resolved with 14,400 nodes.

Finite Volume method for BGK and ES-BGK equations

A finite volume solver SMOKE developed at ERC has been used to deterministically solve the BGK and ES-BGK equations. SMOKE is a parallel code based on conservative numerical schemes developed by L. Mieussens [12]. A second order spatial discretization with axial symmetry is used along with implicit time integration. A supersonic inflow condition is used at the nozzle throat, and vacuum outflow conditions are set at the outer boundaries. Fully diffuse reflection with complete energy accommodation is applied at the nozzle surface. The spatial grid convergence was achieved by increasing the number of nodes from 3,600 to over 17,000. The convergence on the velocity grid is also studied, with the number of (x, r, θ) points ranging from (20,10,18) to (30,35,50).

Statistical method for BGK equation

In our earlier work [13], we had developed and studied a statistical technique, called eDSMC, which models continuum flows through a collision enforcement procedure which guarantees full relaxation of the molecular thermal velocities to the state of local equilibrium. The technique is able to solve inviscid flows with tangency boundary conditions at the wall, but tends to under predict the viscous effects in the boundary layer when diffusional boundary conditions are used. In this work we continue our effort to apply statistical methods to moderate and high Reynolds number nozzle flows by making use of the BGK [3] model.

Recently, a number of authors [5, 14, 6] have developed particle approaches to the solution of the BGK and ES-BGK model equations. The essence of these kinetic approaches is to relax the flow to local Maxwellian or Gaussian equilibrium by choosing a fraction of simulated particles available in a computational cell, and assigning them new velocities according to the local Maxwellian (or ellipsoidal) distribution. If the collision frequency for

such a velocity reassignment is properly computed and local values of the translational temperature in the cell are known, then the procedure should simulate the collision term on the right hand side of the BGK equation,

$$\partial(nf)/\partial t + \vec{c} \cdot \partial(nf)/\partial \vec{r} = \nu n(f_e - f)$$

where n is the number density, ν is the collision frequency, f is the molecular velocity distribution function, f_e is the Maxwellian distribution function, \vec{c} is the velocity vector, and \vec{r} is the position vector.

The details of the statistical BGK scheme are as follows. The collision frequency is calculated as

$$\nu = \text{Pr} \cdot nk \left(\frac{T_{ref}^\omega}{\mu_{ref}} \right) T^{1-\omega}$$

where Pr is the Prandtl number (1 for the BGK equation), k is the Boltzmann constant, T is the translational temperature in the flow, μ_{ref} is the gas dynamic viscosity at T_{ref} . The collision frequency is calculated for each computational cell at each time step based on the local translational temperature T and the local number density n . The local number density n was averaged over a large number of computational time steps, while the local temperature T is computed based on the instantaneous thermal velocities of the computational particles in the cell.

The number of particles in a cell preselected for velocity re-sampling was calculated as follows:

$$N_c = \text{int}(N(1 - \exp(-\nu\Delta t)))$$

where Δt is the time step, N is the number of particles in the cell and int operator means the nearest smaller integer. In order to compensate for the systematic error that such an operator produces, one more particle was added to the list of preselected particles with the probability given by following equation:

$$P_c = N(1 - \exp(-\nu\Delta t)) - \text{int}(N(1 - \exp(-\nu\Delta t)))$$

The preselected particles receive new velocities according to a Maxwellian distribution corresponding to the local cell temperature and velocity. The velocities of particles which have not been preselected remain unchanged in the current timestep.

Although the technique is not limited to simple gases[6], argon was used as the working gas in order to understand the basic features and limitations of the method, avoiding the additional complication of translational-rotational relaxation. In order to reduce the statistical error so that small differences among the different methods may be studied, a large number of simulated particles were used such that the minimum number of particles per cell was about 150. This unusually large number of particles per cell also provided a better statistical approximation of local instantaneous cell based temperature.

RESULTS AND DISCUSSION

Low pressure Case I

The results presented below for the low pressure Case I were obtained by the DSMC code (SMILE), its modification implementing the statistical BGK scheme, a finite volume (FV) ES-BGK solver, and a Navier-Stokes solver, CFD++. To quantify the differences among the different approaches, the gas parameters are presented along two cross sections, the nozzle centerline and the nozzle exit plane. The velocity, and temperature along the centerline are shown in Figs. 1 and 2. Here, $X=0$ corresponds to the nozzle throat. It is evident that all four of our approaches produce very similar results for all gas properties under consideration.

The axial velocity and temperature along the nozzle exit plane are presented in Figs. 3 and 4. Here, $Y=0$ corresponds to the nozzle centerline. The FV ES-BGK solution is close to that of DSMC for both the axial velocity and gas temperature. The particle BGK result agrees well with the FV ES-BGK and DSMC. The NS solver produces results accurate in the coreflow but strongly different from the ES-BGK, DSMC and particle BGK throughout the boundary layer. Generally, we can conclude that the statistical and FV ES-BGK results are in very good agreement with the DSMC in the entire diverging part of the nozzle. The solution of the model kinetic equation accurately captures both the boundary layer and the nozzle coreflow.

High pressure Case II

Results for the high pressure Case II were obtained by the baseline DSMC, statistical BGK scheme, Finite Volume BGK solver, the Navier-Stokes solver and eDSMC method. A quantitative comparison of flow velocity and temperature for Case II is given in Figures. 5 and 6, where the velocity and temperature profiles along the nozzle centerline are shown, and in Figures. 7 and 8 for the velocity and temperature profiles along the nozzle exit plane. It is clearly seen that the DSMC, NS, FV ES-BGK and statistical BGK profiles of both velocity and temperature are very close along the nozzle centerline. The results obtained with eDSMC are similar to particle BGK in the coreflow. The results along the exit plane show that there is still some difference between the NS and DSMC predictions, both in temperature and flow velocity. As in Case I, this difference is explained by the limitations of the velocity slip boundary condition used in NS. There is some impact of flow nonequilibrium too, but its contribution is significant only near the nozzle lip, where T_x/T ratio reaches 0.85.

Tables 1 and 2 show the comparison of computational time required by various methods for low pressure and high pressure cases respectively. It is interesting to note that computational efforts for the DSMC and statistical BGK schemes were of the same order, but the convergence process was quite different. The DSMC schemes tend to converge faster, but requires more computational effort to collect the sufficient information for the solution to be smooth. On the other hand statistical BGK converges slower (perhaps due to the "history" of the macro-parameter sampling procedure which defines the local Maxwellian distribution function), but the smoothness of the results is achieved earlier than in the case of DSMC (probably for the same reason). eDSMC, although very fast (comparable with the NS solver), does not capture the viscous effects in the boundary layer, yet solution in the inviscid core of the flow is remarkably close to the solutions obtained by using other methods.

CONCLUSIONS

Argon flow through a conical nozzle was studied for two Reynolds numbers of 1,230 and 12,300, using four different approaches. These include one continuum approach (solution of Navier-Stokes equations) and three kinetic approaches (the DSMC method, and statistical and deterministic methods for the BGK equation). Analyses of the accuracy of the approaches and their numerical efficiency was conducted. Several conclusions can be drawn from the results of the computations. The most accurate data in both high and low pressure cases was obtained by DSMC even though parameters of the numerical scheme were somewhat relaxed in the high pressure Case II.

The Navier-Stokes solutions are in good agreement with the DSMC results in the higher density portion of the flow and in the coreflow, where rarefaction effects are small. In the boundary layer, even though the velocity slip and temperature jump boundary conditions were used, there is a difference between the NS and DSMC solutions. The statistical and finite volume solution of the ES-BGK equation are in fair agreement with the DSMC method in the entire computational domain for both Reynolds numbers.

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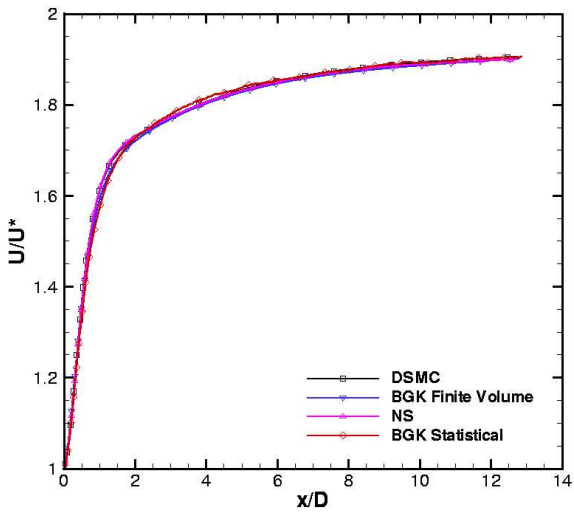


FIGURE 1. Velocity profile along nozzle axis for low pressure case

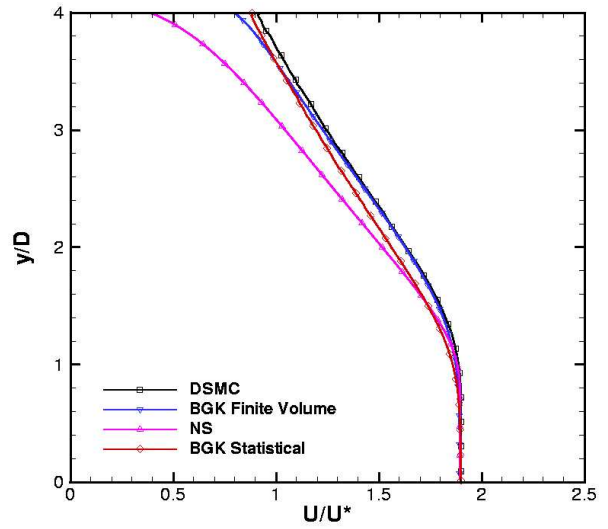


FIGURE 3. Velocity profile at nozzle exit plane for low pressure case

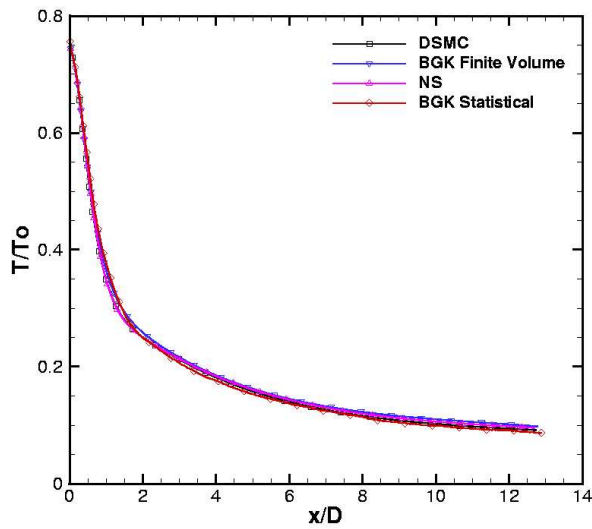


FIGURE 2. Temperature profile along nozzle axis for low pressure case

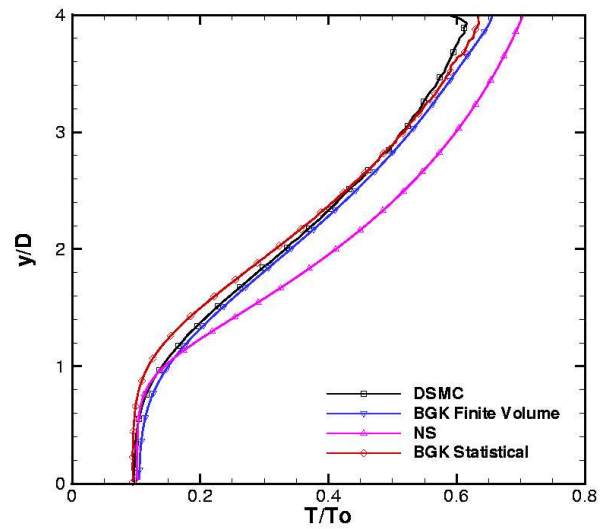


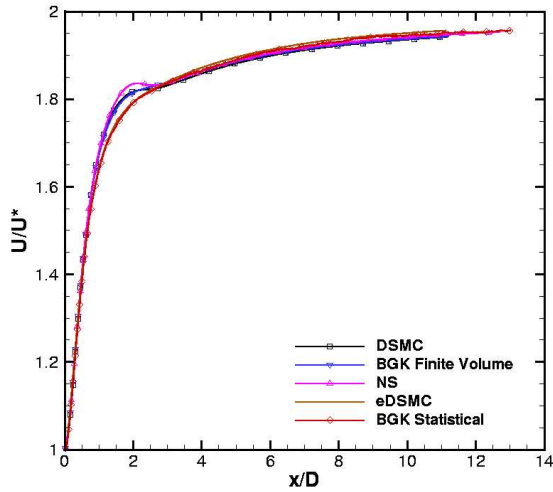
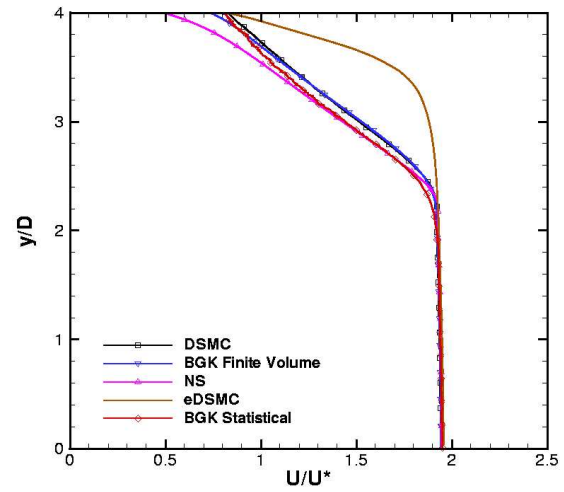
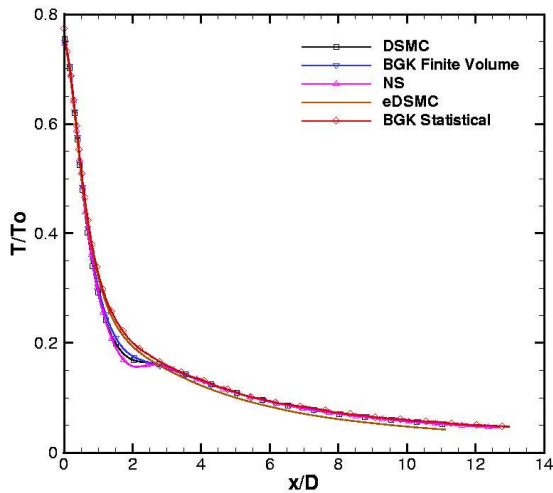
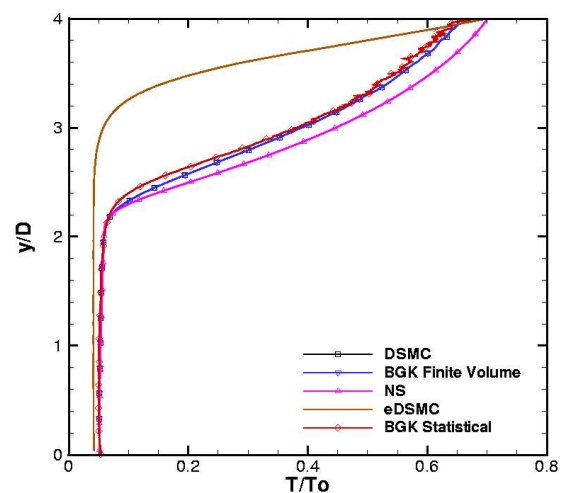
FIGURE 4. Temperature profile at nozzle exit plane for low pressure case

TABLE 1. Parameters of the methods, Case I

Method	DSMC	Part BGK	FV ES-BGK	NS
Time (CPUH)	200	1000	400	<1
Number of particles	10 mil	50 mil	-	-
Number of cells	3 mil	0.5 mil	3,600	3,600

TABLE 2. Parameters of the methods, Case II

Method	DSMC	Part BGK	FV ES-BGK	NS	eDSMC
Time (CPUH)	1000	1000	5000	3	100
Number of particles	50 mil	50 mil	-	-	1 mil
Number of cells	15 mil	0.5 mil	17,200	14,400	100,000

**FIGURE 5.** Velocity profile along nozzle axis for high pressure case**FIGURE 7.** Velocity profile at nozzle exit plane for high pressure case**FIGURE 6.** Temperature profile along nozzle axis for high pressure case**FIGURE 8.** Temperature profile at nozzle exit plane for high pressure case